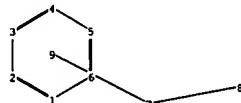
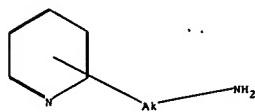


## EAST Search History

Ref #	Hits	Search Query	DBs	Default Operator	Plurals	Time Stamp
L1	1334	((546/290) or (546/334)).CCLS.	US-PGPUB; USPAT	OR	OFF	2007/07/06 10:44
L2	670	1 and amino and methyl and pyridine	US-PGPUB; USPAT	OR	OFF	2007/07/06 11:05
L3	0	("vangelistiadjmanuel.inv.)").PN.	US-PGPUB	OR	OFF	2007/07/06 11:05



chain nodes :

7 8

ring nodes :

1 2 3 4 5 6

chain bonds :

7-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

7-8

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

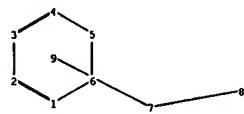
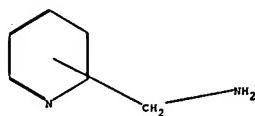
containing 1 :

Connectivity :

7:2 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom



chain nodes :

7 8

ring nodes :

1 2 3 4 5 6

chain bonds :

7-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact bonds :

7-8

normalized bonds :

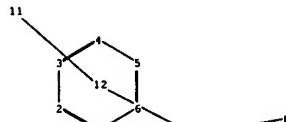
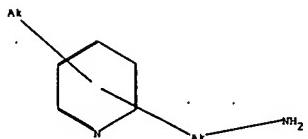
1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom

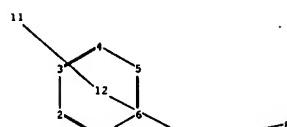
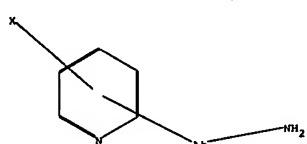


```

chain nodes :
 7 8 11
ring nodes :
 1 2 3 4 5 6
chain bonds :
 7-8
ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
 7-8
normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
 containing 1 :

Connectivity :
 7:2 E exact RC ring/chain
Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom
11:CLASS 12:Atom

```

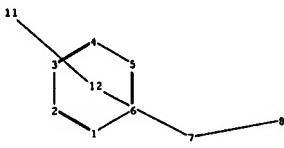
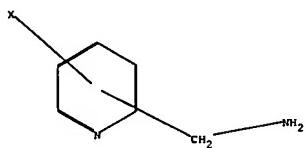


```

chain nodes :
 7 8 11
ring nodes :
 1 2 3 4 5 6
chain bonds :
 7-8
ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
exact/norm bonds :
 7-8
normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
 containing 1 :

Connectivity :
 7:2 E exact RC ring/chain
Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom
11:CLASS 12:Atom

```



chain nodes :

7 8 11

ring nodes :

1 2 3 4 5 6

chain bonds :

7-8

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact bonds :

7-8

normalized bonds :

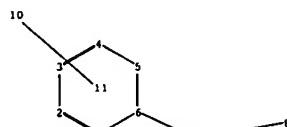
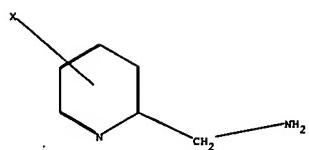
1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 9:Atom  
11:CLASS 12:Atom

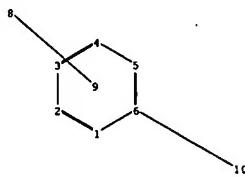
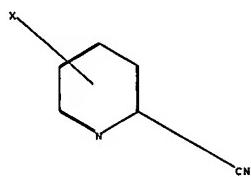


```

chain nodes :
 7 8 10
ring nodes :
 1 2 3 4 5 6
chain bonds :
 6-7 7-8
ring bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
exact bonds :
 6-7 7-8
normalized bonds :
 1-2 1-6 2-3 3-4 4-5 5-6
isolated ring systems :
 containing 1 :

Match level :
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:CLASS 8:CLASS 10:CLASS
 11:Atom

```



chain nodes :

8 10

ring nodes :

1 2 3 4 5 6

chain bonds :

6-10

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact bonds :

6-10

normalized bonds :

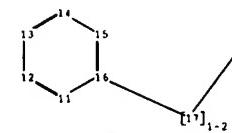
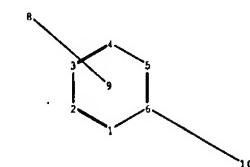
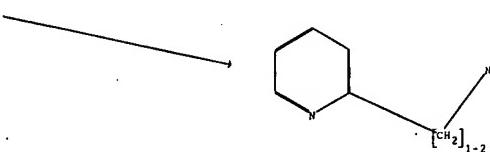
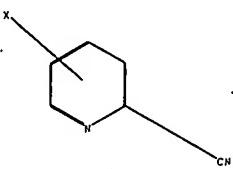
1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:Atom 10:CLASS



chain nodes :

8 10 17 18

ring nodes :

1 2 3 4 5 6 11 12 13 14 15 16

chain bonds :

6-10 16-17 17-18

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

exact bonds :

6-10 16-17 17-18

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 11-12 11-16 12-13 13-14 14-15 15-16

isolated ring systems :

containing 1 : 11 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 8:CLASS 9:Atom 10:CLASS  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS

fragments assigned reactant role:

containing 1

fragments assigned product role:

containing 11

10535723

## Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1612bxr

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

NEWS 1 Web Page for STN Seminar Schedule - N. America  
NEWS 2 MAR 15 WPIDS/WPIX enhanced with new FRAGHITSTR display format  
NEWS 3 MAR 16 CASREACT coverage extended  
NEWS 4 MAR 20 MARPAT now updated daily  
NEWS 5 MAR 22 LWPII reloaded  
NEWS 6 MAR 30 RDISCLOSURE reloaded with enhancements  
NEWS 7 APR 02 JICST-EPLUS removed from database clusters and STN  
NEWS 8 APR 30 GENBANK reloaded and enhanced with Genome Project ID field.  
NEWS 9 APR 30 CHEMCATS enhanced with 1.2 million new records  
NEWS 10 APR 30 CA/CAplus enhanced with 1870-1889 U.S. patent records  
NEWS 11 APR 30 INPADOC replaced by INPADOCDB on STN  
NEWS 12 MAY 01 New CAS web site launched  
NEWS 13 MAY 08 CA/CAplus Indian patent publication number format defined  
NEWS 14 MAY 14 RDISCLOSURE on STN Easy enhanced with new search and display fields  
NEWS 15 MAY 21 BIOSIS reloaded and enhanced with archival data  
NEWS 16 MAY 21 TOXCENTER enhanced with BIOSIS reload  
NEWS 17 MAY 21 CA/CAplus enhanced with additional kind codes for German patents  
NEWS 18 MAY 22 CA/CAplus enhanced with IPC reclassification in Japanese patents  
NEWS 19 JUN 27 CA/CAplus enhanced with pre-1967 CAS Registry Numbers  
NEWS 20 JUN 29 STN Viewer now available  
NEWS 21 JUN 29 STN Express, Version 8.2, now available  
NEWS 22 JUL 02 LEMBASE coverage updated  
NEWS 23 JUL 02 LMEDLINE coverage updated  
NEWS 24 JUL 02 SCISEARCH enhanced with complete author names  
NEWS 25 JUL 02 CHEMCATS accession numbers revised  
NEWS 26 JUL 02 CA/CAplus enhanced with utility model patents from China

NEWS EXPRESS 29 JUNE 2007: CURRENT WINDOWS VERSION IS V8.2,  
CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP),  
AND CURRENT DISCOVER FILE IS DATED 4 MAY 2007.

NEWS HOURS STN Operating Hours Plus Help Desk Availability  
NEWS LOGIN Welcome Banner and News Items  
NEWS IBC8 For general information regarding STN implementation of IBC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 11:12:22 ON 06 JUL 2007

$\Rightarrow$

=> file req

COST IN U.S. DOLLARS

SINCE FILE ENTRY	TOTAL SESSION
0.21	0.21

FULL ESTIMATED COST

FILE 'REGISTRY' ENTERED AT 11:12:38 ON 06 JUL 2007

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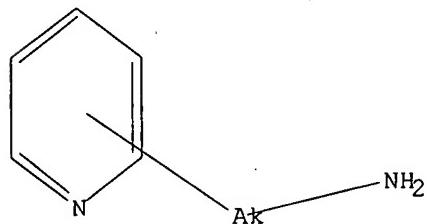
=>  
Uploading C:\Documents and Settings\brobins1\My  
Documents\stnweb\Queries\2a323f.str

## L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



## Updated Search

10535723

Structure attributes must be viewed using STN Express query preparation.

=> s 11  
SAMPLE SEARCH INITIATED 11:14:24 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 150568 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

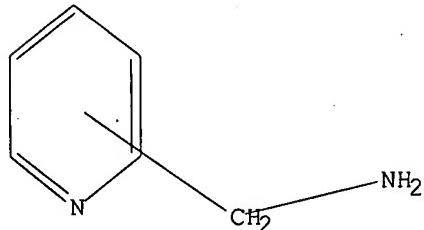
FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 2988464 TO 3034256  
PROJECTED ANSWERS: 9162 TO 11916

L2 7 SEA SSS SAM L1

=>  
Uploading C:\Documents and Settings\brobinson1\My  
Documents\stnweb\Queries\rererh.str

L3 STRUCTURE UPLOADED

=> d 13  
L3 HAS NO ANSWERS  
L3 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 13  
SAMPLE SEARCH INITIATED 11:15:10 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 150568 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 2988464 TO 3034256  
PROJECTED ANSWERS: 7759 TO 10309

L4 6 SEA SSS SAM L3

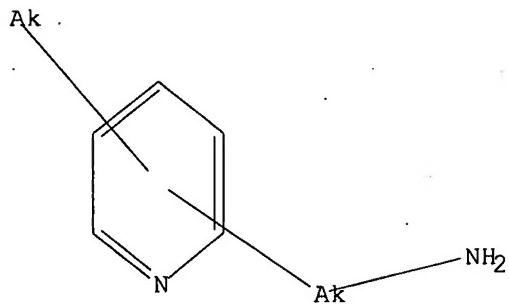
=>  
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\qwj.str

Updated Search

10535723

L5 STRUCTURE UPLOADED

=> d 15  
L5 HAS NO ANSWERS  
L5 STR



Structure attributes must be viewed using STN Express query preparation.

=> s 15  
SAMPLE SEARCH INITIATED 11:16:58 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 150568 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS 4 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 2988464 TO 3034256  
PROJECTED ANSWERS: 4981 TO 7063

L6 4 SEA SSS SAM L5

=>  
Uploading C:\Documents and Settings\brobins01\My Documents\stnweb\Queries\erern.str

L7 STRUCTURE UPLOADED

=> s 17  
SAMPLE SEARCH INITIATED 11:17:38 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 150568 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS 0 ANSWERS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 2988464 TO 3034256  
PROJECTED ANSWERS: 0 TO 0

L8 0 SEA SSS SAM L7

Updated Search

10535723

=>  
Uploading C:\Documents and Settings\brobinsone\My Documents\stnweb\Queries\qmh.str

L9 STRUCTURE uploaded

=> s 19  
SAMPLE SEARCH INITIATED 11:18:21 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 150568 TO ITERATE

1.3% PROCESSED 2000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 2988464 TO 3034256  
PROJECTED ANSWERS: 0 TO 0

L10 0 SEA SSS SAM L9

=>  
Uploading C:\Documents and Settings\brobinsone\My Documents\stnweb\Queries\rmgy.str

L11 STRUCTURE uploaded

=> s 111  
SAMPLE SEARCH INITIATED 11:19:11 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 9663 TO ITERATE

20.7% PROCESSED 2000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 187369 TO 199151  
PROJECTED ANSWERS: 7 TO 379

L12 2 SEA SSS SAM L11

=> s 111 full  
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
FULL SEARCH INITIATED 11:19:15 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 192512 TO ITERATE

100.0% PROCESSED 192512 ITERATIONS 66 ANSWERS  
SEARCH TIME: 00.00.01

L13 66 SEA SSS FUL L11

=> file hcplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 176.60 176.81

FILE 'HCPLUS' ENTERED AT 11:19:19 ON 06 JUL 2007  
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FILE COVERS 1907 - 6 Jul 2007 VOL 147 ISS 3  
FILE LAST UPDATED: 5 Jul 2007 (20070705/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s 113  
L14 89 L13

=> s 1113/prep  
L113 NOT FOUND  
The L-number entered has not been defined in this session, or it has been deleted. To see the L-numbers currently defined in this session, enter DISPLAY HISTORY at an arrow prompt (>).

=> s 113/prep  
89 L13  
4427949 PREP/RL  
L15 57 L13/PREP  
(L13 (L) PREP/RL)

	SINCE FILE	TOTAL
	ENTRY	SESSION
COST IN U.S. DOLLARS		
FULL ESTIMATED COST	2.60	179.41

FILE 'REGISTRY' ENTERED AT 11:19:38 ON 06 JUL 2007  
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<http://www.cas.org/support/stngen/stndoc/properties.html>

=>  
Uploading C:\Documents and Settings\brobinsone\My Documents\stnweb\Queries\oki7.str

L16 STRUCTURE UPLOADED

=> s 116  
SAMPLE SEARCH INITIATED 11:20:38 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 950 TO ITERATE

100.0% PROCESSED 950 ITERATIONS 13 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 17151 TO 20849  
PROJECTED ANSWERS: 44 TO 476

L17 13 SEA SSS SAM L16

=> s 116 full  
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 171.65 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
FULL SEARCH INITIATED 11:20:43 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 17958 TO ITERATE

100.0% PROCESSED 17958 ITERATIONS 338 ANSWERS  
SEARCH TIME: 00.00.01

L18 338 SEA SSS FUL L16

=> file hcaplus  
COST IN U.S. DOLLARS SINCE FILE TOTAL  
ENTRY SESSION  
FULL ESTIMATED COST 172.55 351.96

FILE 'HCAPLUS' ENTERED AT 11:20:46 ON 06 JUL 2007  
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```
=> s 118/rct
      560 L18
      2989518 RCT/RL
L19      455 L18/RCT
          (L18 (L) ·RCT/RL)
```

```
=> d his
```

(FILE 'HOME' ENTERED AT 11:12:22 ON 06 JUL 2007)

FILE 'REGISTRY' ENTERED AT 11:12:38 ON 06 JUL 2007

```
L1      STRUCTURE uploaded
L2      7 S L1
L3      STRUCTURE uploaded
L4      6 S L3
L5      STRUCTURE uploaded
L6      4 S L5
L7      STRUCTURE uploaded
L8      0 S L7
L9      STRUCTURE uploaded
L10     0 S L9
L11     STRUCTURE uploaded
L12     2 S L11
L13     66 S L11 FULL
```

FILE 'HCAPLUS' ENTERED AT 11:19:19 ON 06 JUL 2007

```
L14     89 S L13
L15     57 S L13/PREP
```

FILE 'REGISTRY' ENTERED AT 11:19:38 ON 06 JUL 2007

```
L16     STRUCTURE uploaded
L17     13 S L16
L18     338 S L16 FULL
```

FILE 'HCAPLUS' ENTERED AT 11:20:46 ON 06 JUL 2007

```
L19     455 S L18/RCT
```

```
=> s 119 and 115
L20     36 L19 AND L15
```

```
=> file reg
COST IN U.S. DOLLARS           SINCE FILE      TOTAL
                                ENTRY          SESSION
FULL ESTIMATED COST          2.60          354.56
```

FILE 'REGISTRY' ENTERED AT 11:21:03 ON 06 JUL 2007  
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DICTIONARY FILE UPDATES: 5 JUL 2007 HIGHEST RN 941372-96-9

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<http://www.cas.org/support/stngen/stndoc/properties.html>

```
=> e nickel/rn
E1      1    99999-98-1/RN
E2      1    99999-99-2/RN
E3      0 --> NICKEL/RN
***** END OF FIELD *****

=> e nickel/cn
E1      1    NICKASE TRAA (PLASMID PLW1071) GENE TRAA)/CN
E2      1    NICKASE-HELICASE (PLASMID TI PLASMID PTI15955 GENE TRAA)/CN
E3      1 --> NICKEL/CN
E4      1    NICKEL (0), BIS(METHANETRICARBONITRILATO)DINITROSYLBIS(TRICYCLOHEXYLPHOSPHINE)DI-/CN
E5      1    NICKEL (1+) ACETYLACETONATE/CN
E6      1    NICKEL (1+), HYDROTRIS(TRIETHYLPHOSPHINE)-/CN
E7      1    NICKEL (19.2-31.0), ZINC (69.0-80.8) (ATOMIC)/CN
E8      1    NICKEL (2+) ORTHOPHOSPHATE OCTAHYDRATE/CN
E9      1    NICKEL (2+), HEXAAMMINE-, BIS(METABORATE)/CN
E10     1    NICKEL (25.6), TIN (1.5), ZINC (72.9) (ATOMIC)/CN
E11     1    NICKEL (58NI1+)/CN
E12     1    NICKEL (ADENINE) DIBROMIDE/CN
```

```
=> s e3
L21      1 NICKEL/CN
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=> file hcaplus
COST IN U.S. DOLLARS          SINCE FILE      TOTAL
                                ENTRY           SESSION
FULL ESTIMATED COST          5.40            359.96
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FILE 'HCAPLUS' ENTERED AT 11:21:21 ON 06 JUL 2007  
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FILE COVERS 1907 - 6 Jul 2007 VOL 147 ISS 3  
FILE LAST UPDATED: 5 Jul 2007 (20070705/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l21  
L22 342935 L21

=> s l21/cat  
342935 L21  
631560 CAT/RL  
L23 34808 L21/CAT  
(L21 (L) CAT/RL)

=> s l21/catalyst  
'CATALYST' IS NOT A VALID CROSSOVER QUALIFIER FOR L21  
Answer sets created in a different file may be field qualified with a limited set of qualifiers. Enter HELP CROSSOVER at an arrow prompt (=>) for specific information.

=> d his

(FILE 'HOME' ENTERED AT 11:12:22 ON 06 JUL 2007)

FILE 'REGISTRY' ENTERED AT 11:12:38 ON 06 JUL 2007  
L1 STRUCTURE UPLOADED  
L2 7 S L1  
L3 STRUCTURE UPLOADED  
L4 6 S L3  
L5 STRUCTURE UPLOADED  
L6 4 S L5  
L7 STRUCTURE UPLOADED  
L8 0 S L7  
L9 STRUCTURE UPLOADED  
L10 0 S L9  
L11 STRUCTURE UPLOADED  
L12 2 S L11  
L13 66 S L11 FULL

FILE 'HCAPLUS' ENTERED AT 11:19:19 ON 06 JUL 2007  
L14 89 S L13  
L15 57 S L13/PREP

FILE 'REGISTRY' ENTERED AT 11:19:38 ON 06 JUL 2007  
L16 STRUCTURE UPLOADED  
L17 13 S L16  
L18 338 S L16 FULL

FILE 'HCAPLUS' ENTERED AT 11:20:46 ON 06 JUL 2007  
L19 455 S L18/RCT  
L20 36 S L19 AND L15

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FILE 'REGISTRY' ENTERED AT 11:21:03 ON 06 JUL 2007

E NICKEL/RN  
E NICKEL/CN

L21 1 S E3

FILE 'HCAPLUS' ENTERED AT 11:21:21 ON 06 JUL 2007

L22 342935 S L21  
L23 34808 S L21/CAT

=> s 122 and 123

L24 34808 L22 AND L23

=> s 122 and 120

L25 2 L22 AND L20

=> d 125, ibib abs hitstr, 1-2

L25 ANSWER 1 OF 2 HCAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2004:427623 HCAPLUS

DOCUMENT NUMBER: 141:7024

TITLE: A novel process for the preparation of  
2-aminomethylpyridine derivatives via Ni-catalyzed  
hydrogenation of 2-cyanopyridine derivatives

INVENTOR(S): Vangelisti, Manuel

PATENT ASSIGNEE(S): Bayer Cropscience Sa, Fr.

SOURCE: Eur. Pat. Appl., 6 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

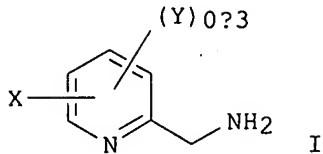
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1422221	A1	20040526	EP 2002-356236	20021120
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
WO 2004046114	A1	20040603	WO 2003-EP14892	20031118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003290121	A1	20040615	AU 2003-290121	20031118
BR 2003014461	A	20050726	BR 2003-14461	20031118
EP 1565440	A1	20050824	EP 2003-782483	20031118
EP 1565440	B1	20061220		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1711244	A	20051221	CN 2003-80103328	20031118
JP 2006508143	T	20060309	JP 2004-552709	20031118
AT 348811	T	20070115	AT 2003-782483	20031118
US 2006004206	A1	20060105	US 2005-535723	20050520
PRIORITY APPLN. INFO.:			EP 2002-356236	A 20021120

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OTHER SOURCE(S):  
GI

WO 2003-EP14892  
CASREACT 141:7024; MARPAT 141:7024

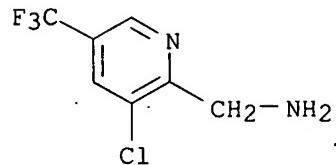
W 20031118



- AB The invention relates to a process for the preparation of 2-aminomethylpyridine derivs. of formula I [wherein: X is halogen atom; each Y may be the same or different and may be a halogen atom, a halogenoalkyl, an alkoxy carbonyl or an alkylsulfonyl], useful as intermediates for preparation of pesticides. 2-Aminomethyl-3-chloro-5-trifluoromethylpyridine was prepared via Raney Ni-catalyzed hydrogenation of 2-cyano-3-chloro-5-trifluoromethylpyridine with a yield of 97%. The advantages of the proposed preparation of 2-aminomethylpyridine derivs. include the use of Raney nickel catalyst instead of expensive Pd catalyst (the Pd-catalyzed hydrogenation suffers from the disadvantage of dehalogenation reaction; Pd is also very sensitive to catalyst poisons).
- IT 7440-02-0, Raney nickel, uses  
RL: CAT (Catalyst use); USES (Uses)  
(catalysts; novel process for the preparation of aminomethylpyridine derivs. via Raney Ni-catalyzed hydrogenation of cyanopyridine derivs.)
- RN 7440-02-0 HCAPLUS
- CN Nickel (CA INDEX NAME)

Ni

- IT 175277-74-4P  
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
(novel process for the preparation of aminomethylpyridine derivs. via Raney Ni-catalyzed hydrogenation of cyanopyridine derivs.)
- RN 175277-74-4 HCAPLUS
- CN 2-Pyridinemethanamine, 3-chloro-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)

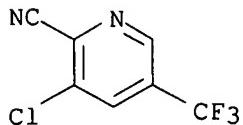


- IT 80194-70-3  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reactant; novel process for the preparation of aminomethylpyridine derivs.)

Updated Search

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via Raney Ni-catalyzed hydrogenation of cyanopyridine derivs.)  
RN 80194-70-3 HCPLUS  
CN 2-Pyridinecarbonitrile, 3-chloro-5-(trifluoromethyl)- (9CI) (CA INDEX  
NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 2 OF 2 HCPLUS COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 2002:157737 HCPLUS  
DOCUMENT NUMBER: 136:200109  
TITLE: Process for preparation of 2-aminomethylpyridines by catalytic hydrogenation of 2-cyanopyridines.  
INVENTOR(S): Dann, Norman; Riordan, Peter Dominic; Amin, Mehul Rasikchandra; Mellor, Michael  
PATENT ASSIGNEE(S): Aventis CropScience SA, Fr.  
SOURCE: PCT Int. Appl., 18 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002016322	A2	20020228	WO 2001-EP10984	20010821
WO 2002016322	A3	20020606		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1199305	A1	20020424	EP 2001-420128	20010607
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CA 2415842	A1	20020228	CA 2001-2415842	20010821
AU 200213948	A	20020304	AU 2002-13948	20010821
EP 1311483	A2	20030521	EP 2001-982337	20010821
EP 1311483	B1	20061220		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001013259	A	20030715	BR 2001-13259	20010821
JP 2004506716	T	20040304	JP 2002-521198	20010821
RU 2266900	C2	20051227	RU 2003-107931	20010821
CN 1721406	A	20060118	CN 2005-10088220	20010821
AT 348810	T	20070115	AT 2001-982337	20010821
EP 1746089	A1	20070124	EP 2006-120806	20010821

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NL, PT, SE, TR

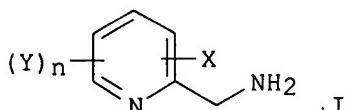
IN 2003MN00064	A	20050204	IN 2003-MN64	20030113
US 2004049048	A1	20040311	US 2003-362728	20030611
US 6921828	B2	20050726		
US 2005250947	A1	20051110	US 2005-177118	20050708

PRIORITY APPLN. INFO.:

GB 2000-21066	A	20000825
GB 2000-25616	A	20001019
EP 2001-420128	A	20010607
CN 2001-814622	A3	20010821
EP 2001-982337	A3	20010821
WO 2001-EP10984	W	20010821
US 2003-362728	A1	20030611

OTHER SOURCE(S): CASREACT 136:200109; MARPAT 136:200109

GI



AB Title compds. (I; X = halo; Y = halo, haloalkyl, alkoxy carbonyl, alkylsulfonyl; n = 0-3) were prepared by catalytic hydrogenation of the corresponding 2-cyano derivs. Thus, 3-chloro-2-cyano-5-trifluoromethylpyridine (preparation given) was hydrogenated in MeOH over Pd/C containing HCl at 1 atmospheric to give 95-97% 2-aminomethyl-3-chloro-5-trifluoromethylpyridine hydrochloride.

IT 7440-02-0, Nickel, uses

RL: CAT (Catalyst use); USES (Uses)  
(process for preparation of 2-aminomethylpyridines by catalytic hydrogenation of 2-cyanopyridines)

RN 7440-02-0 HCPLUS

CN Nickel (CA INDEX NAME)

Ni

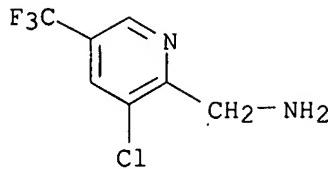
IT 326476-49-7P, 2-Aminomethyl-3-chloro-5-trifluoromethylpyridine hydrochloride

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
(process for preparation of 2-aminomethylpyridines by catalytic hydrogenation of 2-cyanopyridines)

RN 326476-49-7 HCPLUS

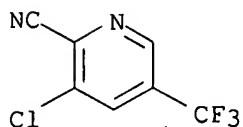
CN 2-Pyridinemethanamine, 3-chloro-5-(trifluoromethyl)-, hydrochloride (1:1)  
(CA INDEX NAME)

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● HCl

IT 80194-70-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP  
(Preparation); RACT (Reactant or reagent)  
(process for preparation of 2-aminomethylpyridines by catalytic  
hydrogenation of 2-cyanopyridines)  
RN 80194-70-3 HCPLUS  
CN 2-Pyridinecarbonitrile, 3-chloro-5-(trifluoromethyl)- (9CI) (CA INDEX  
NAME)



=> file caold			
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION	
FULL ESTIMATED COST	13.14	373.10	
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION	
CA SUBSCRIBER PRICE	-1.56	-1.56	

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FILE COVERS 1907-1966  
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

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more information.

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L1 STRUCTURE uploaded  
L2 7 S L1  
L3 STRUCTURE uploaded  
L4 6 S L3  
L5 STRUCTURE uploaded  
L6 4 S L5  
L7 STRUCTURE uploaded  
L8 0 S L7  
L9 STRUCTURE uploaded  
L10 0 S L9  
L11 STRUCTURE uploaded  
L12 2 S L11  
L13 66 S L11 FULL

FILE 'HCAPLUS' ENTERED AT 11:19:19 ON 06 JUL 2007

L14 89 S L13  
L15 57 S L13/PREP

FILE 'REGISTRY' ENTERED AT 11:19:38 ON 06 JUL 2007

L16 STRUCTURE uploaded  
L17 13 S L16  
L18 338 S L16 FULL

FILE 'HCAPLUS' ENTERED AT 11:20:46 ON 06 JUL 2007

L19 455 S L18/RCT  
L20 36 S L19 AND L15

FILE 'REGISTRY' ENTERED AT 11:21:03 ON 06 JUL 2007

E NICKEL/RN  
E NICKEL/CN  
L21 1 S E3

FILE 'HCAPLUS' ENTERED AT 11:21:21 ON 06 JUL 2007

L22 342935 S L21  
L23 34808 S L21/CAT  
L24 34808 S L22 AND L23  
L25 2 S L22 AND L20

FILE 'CAOLD' ENTERED AT 11:22:10 ON 06 JUL 2007

=> s l22 and l20  
QUALIFICATION NOT VALID FOR L18  
Field code qualifications can only be applied to text  
terms.

=> s l18 and l21  
10 L18  
0 L21  
L26 0 L18 AND L21

=> file casreact  
COST IN U.S. DOLLARS SINCE FILE TOTAL

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	ENTRY	SESSION
FULL ESTIMATED COST	0.45	373.55
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-1.56

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FILE CONTENT:1840 - 30 Jun 2007 VOL 147 ISS 2

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\*\*\*\*\*  
\*  
\* CASREACT now has more than 12 million reactions \*  
\*  
\*\*\*\*\*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>  
Uploading C:\Documents and Settings\brobinson1\My Documents\stnweb\Queries\zx.str

L27 STRUCTURE UPLOADED

=> s 127  
SAMPLE SEARCH INITIATED 11:24:40 FILE 'CASREACT'  
SCREENING COMPLETE - 332 REACTIONS TO VERIFY FROM 49 DOCUMENTS  
100.0% DONE 332 VERIFIED 1 HIT RXNS 1 DOCS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED VERIFICATIONS: 5548 TO 7732  
PROJECTED ANSWERS: 1 TO 79

L28 1 SEA SSS SAM L27 ( 1 REACTIONS)

=> s 127 full  
THE ESTIMATED SEARCH COST FOR FILE 'CASREACT' IS 113.10 U.S. DOLLARS  
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y  
FULL SEARCH INITIATED 11:24:47 FILE 'CASREACT'  
SCREENING COMPLETE - 7961 REACTIONS TO VERIFY FROM 1065 DOCUMENTS

100.0% DONE 7961 VERIFIED 11 HIT RXNS 7 DOCS

Updated Search

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SEARCH TIME: 00.00.05

L29            7 SEA SSS FUL L27 (     11 REACTIONS)

=> d 129, ibib abs hitrxn, 1-7  
'HITRXN' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS ----- GI and AB  
ALL ----- BIB, AB, IND, RE, Single-step Reactions  
APPS ----- AI, PRAI  
BIB ----- AN, plus Bibliographic Data  
CAN ----- List of CA abstract numbers without answer numbers  
CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels  
IBIB ----- BIB, indented with text labels  
IND ----- Indexing data  
IPC ----- International Patent Classifications  
ISTD ----- STD, indented with text labels  
OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels  
  
SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations  
  
MAX ----- Same as ALL  
PAT5 ----- PI, SO  
SCAN ----- TI and FCRD (random display, no answer number. SCAN  
              must be entered on the same line as DISPLAY, e.g.,  
              D SCAN.)  
SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for  
              all single-step reactions)  
STD ----- BIB, IPC, and NCL  
  
CRD ----- Compact Display of All Hit Reactions  
CRDREF ----- Compact Reaction Display and SO, PY for Reference  
FHIT ----- Reaction Map, Diagram, and Summary for first  
              hit reaction  
FHITCBIB --- FHIT, AN plus CBIB  
FCRD ----- First hit in Compact Reaction Display (CRD) format  
FCRDREF ----- First hit in Compact Reaction Display (CRD) format with  
              CA reference information (SO, PY). (Default)  
FPATH ----- PATH, plus Reaction Summary for the "long path"  
FSPATH ----- SPATH, plus Reaction Summary for the "short path"  
HIT ----- Reaction Map, Reaction Diagram, and Reaction  
              Summary for all hit reactions and fields containing  
              hit terms  
OCC ----- All hit fields and the number of occurrences of the  
              hit terms in each field. Includes total number of  
              HIT, PATH, SPATH reactions. Labels reactions that have  
              incomplete verifications.  
PATH ----- Reaction Map and Reaction Diagram for the "long  
              path". Displays all hit reactions, except those  
              whose steps are totally included within another hit  
              reaction which is displayed  
RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)

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RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
RXS ----- Hit Reaction Summariers (Map and Summary for all hit reactions)  
SPATH ----- Reaction Map and Reaction Diagram for the "short path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (>). Examples of combinations include: D TI, D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):d his  
'D' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS ----- GI and AB  
ALL ----- BIB, AB, IND, RE, Single-step Reactions  
APPS ----- AI, PRAI  
BIB ----- AN, plus Bibliographic Data  
CAN ----- List of CA abstract numbers without answer numbers  
CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels  
IBIB ----- BIB, indented with text labels  
IND ----- Indexing data  
IPC ----- International Patent Classifications  
ISTD ----- STD, indented with text labels  
OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels  
  
SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations  
  
MAX ----- Same as ALL  
PAT5 ----- PI, SO  
SCAN ----- TI and FCRD (random display, no answer number. SCAN must be entered on the same line as DISPLAY, e.g., D SCAN.)  
SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for all single-step reactions)  
STD ----- BIB, IPC, and NCL  
  
CRD ----- Compact Display of All Hit Reactions  
CRDREF ----- Compact Reaction Display and SO, PY for Reference  
FHIT ----- Reaction Map, Diagram, and Summary for first hit reaction  
FHITCBIB --- FHIT, AN plus CBIB  
FCRD ----- First hit in Compact Reaction Display (CRD) format

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FCRDREF ----- First hit in Compact Reaction Display (CRD) format with CA reference information (SO, PY). (Default)  
FPATH ----- PATH, plus Reaction Summary for the "long path"  
FSPATH ----- SPATH, plus Reaction Summary for the "short path"  
HIT ----- Reaction Map, Reaction Diagram, and Reaction Summary for all hit reactions and fields containing hit terms  
OCC ----- All hit fields and the number of occurrences of the hit terms in each field. Includes total number of HIT, PATH, SPATH reactions. Labels reactions that have incomplete verifications.  
PATH ----- Reaction Map and Reaction Diagram for the "long path". Displays all hit reactions, except those whose steps are totally included within another hit reaction which is displayed  
RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)  
RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
RXS ----- Hit Reaction Summariers (Map and Summary for all hit reactions)  
SPATH ----- Reaction Map and Reaction Diagram for the "short path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI, D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):end

=> d his

(FILE 'HOME' ENTERED AT 11:12:22 ON 06 JUL 2007)

FILE 'REGISTRY' ENTERED AT 11:12:38 ON 06 JUL 2007

L1	STRUCTURE UPLOADED
L2	7 S L1
L3	STRUCTURE UPLOADED
L4	6 S L3
L5	STRUCTURE UPLOADED
L6	4 S L5
L7	STRUCTURE UPLOADED
L8	0 S L7
L9	STRUCTURE UPLOADED
L10	0 S L9
L11	STRUCTURE UPLOADED
L12	2 S L11
L13	66 S L11 FULL

FILE 'HCAPLUS' ENTERED AT 11:19:19 ON 06 JUL 2007

L14 89 S L13

Updated Search

10535723

L15 57 S L13/PREP

FILE 'REGISTRY' ENTERED AT 11:19:38 ON 06 JUL 2007

L16 STRUCTURE UPLOADED

L17 13 S L16

L18 338 S L16 FULL

FILE 'HCAPLUS' ENTERED AT 11:20:46 ON 06 JUL 2007

L19 455 S L18/RCT

L20 36 S L19 AND L15

FILE 'REGISTRY' ENTERED AT 11:21:03 ON 06 JUL 2007

E NICKEL/RN

E NICKEL/CN

L21 1 S E3

FILE 'HCAPLUS' ENTERED AT 11:21:21 ON 06 JUL 2007

L22 342935 S L21

L23 34808 S L21/CAT

L24 34808 S L22 AND L23

L25 2 S L22 AND L20

FILE 'CAOLD' ENTERED AT 11:22:10 ON 06 JUL 2007

L26 0 S L18 AND L21

FILE 'CASREACT' ENTERED AT 11:22:48 ON 06 JUL 2007

L27 STRUCTURE UPLOADED

L28 1 S L27

L29 7 S L27 FULL

=> d 129, ibib abs fhit, 1-7

L29 ANSWER 1 OF 7 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 144:331318 CASREACT

TITLE: Biological evaluation of isothiazoloquinolones containing aromatic heterocycles at the 7-position: In vitro activity of a series of potent antibacterial agents that are effective against methicillin-resistant *Staphylococcus aureus*

AUTHOR(S): Wiles, Jason A.; Song, Yongsheng; Wang, Qiuping; Lucien, Edlaine; Hashimoto, Akihiro; Cheng, Jijun; Marlor, Christopher W.; Ou, Yangsi; Podos, Steven D.; Thanassi, Jane A.; Thoma, Christy L.; Deshpande, Milind; Pucci, Michael J.; Bradbury, Barton J.

CORPORATE SOURCE: Achillion Pharmaceuticals, Inc., New Haven, CT, 06511-6653, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2006), 16(5), 1277-1281

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier B.V.

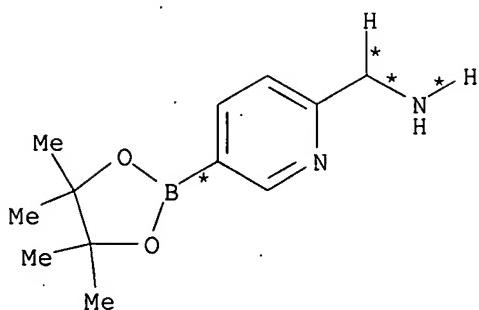
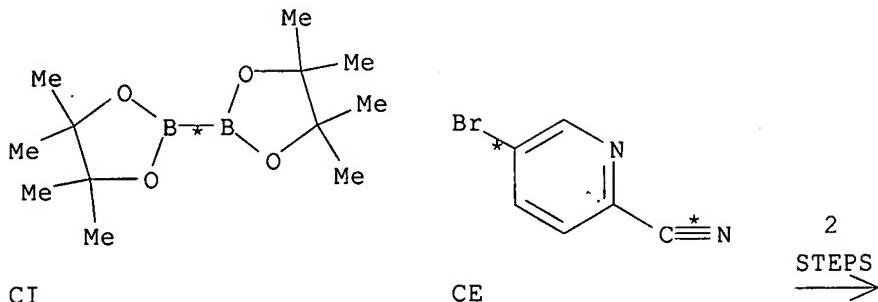
DOCUMENT TYPE: Journal

LANGUAGE: English

AB A diverse series of 9H-isothiazolo[5,4-b]quinoline-3,4-diones containing heteroarom. groups at the 7-position was prepared via palladium-catalyzed cross-coupling. Many of these compds. demonstrated potent antistaphylococcal activity (MICs  $\leq$ 2  $\mu$ g/mL) against a multi-drug-resistant strain (ATCC 700699) and low cytotoxic activity (CC50  $>$  100  $\mu$ M) against the human cell line Hep2 (laryngeal carcinoma).

10535723

RX(46) OF 56 COMPOSED OF RX(40), RX(41)  
RX(46) CI + CE ==> AD



AD  
YIELD 100%

RX(40) RCT CI 73183-34-3, CE 97483-77-7  
RGT CK 127-08-2 AcOK  
PRO CJ 741709-63-7  
CAT 72287-26-4 Palladium, [1,1'-bis(diphenylphosphino-  
κP)ferrocene]dichloro-, (SP-4-2)-  
SOL 67-68-5 DMSO  
CON 25 hours, 80 deg C

RX(41)	RCT	CJ 741709-63-7
	RGT	CN 1333-74-0 H2
	PRO	AD 880495-82-9
	CAT	7440-05-3 Pd
	SOL	64-19-7 AcOH
	CON	16 hours, room temperature

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 2 OF 7 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 142:240471 CASREACT

**TITLE:** Preparation of benzodiazepine derivatives as CGRP receptor antagonists

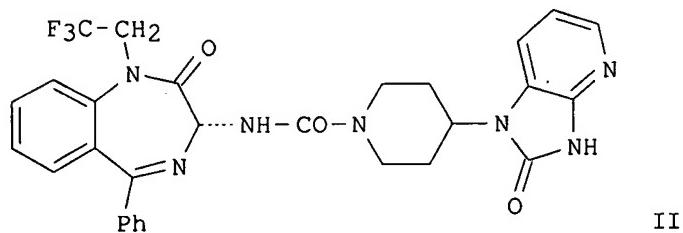
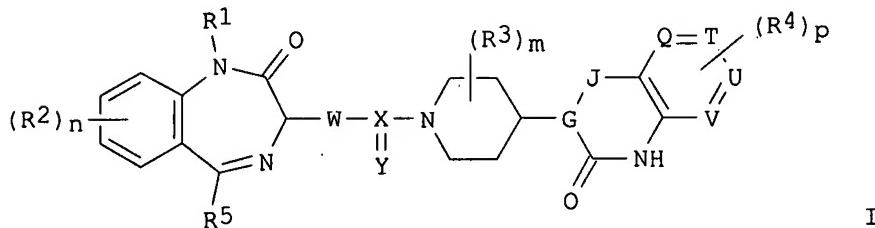
10535723

INVENTOR(S): Burgey, Christopher S.; Stump, Craig A.; Williams, Theresa M.  
PATENT ASSIGNEE(S): Merck & Co., Inc., USA  
SOURCE: PCT Int. Appl., 79 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005013894	A2	20050217	WO 2004-US20209	20040624
WO 2005013894	A3	20060302		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2004263080	A1	20050217	AU 2004-263080	20040624
CA 2529196	A1	20050217	CA 2004-2529196	20040624
EP 1641423	A2	20060405	EP 2004-776997	20040624
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1842526	A	20061004	CN 2004-80017996	20040624
JP 2007516183	T	20070621	JP 2006-517599	20040624
US 2006135511	A1	20060622	US 2005-562297	20051222
PRIORITY APPLN. INFO.:			US 2003-482854P	20030626
			WO 2004-US20209	20040624

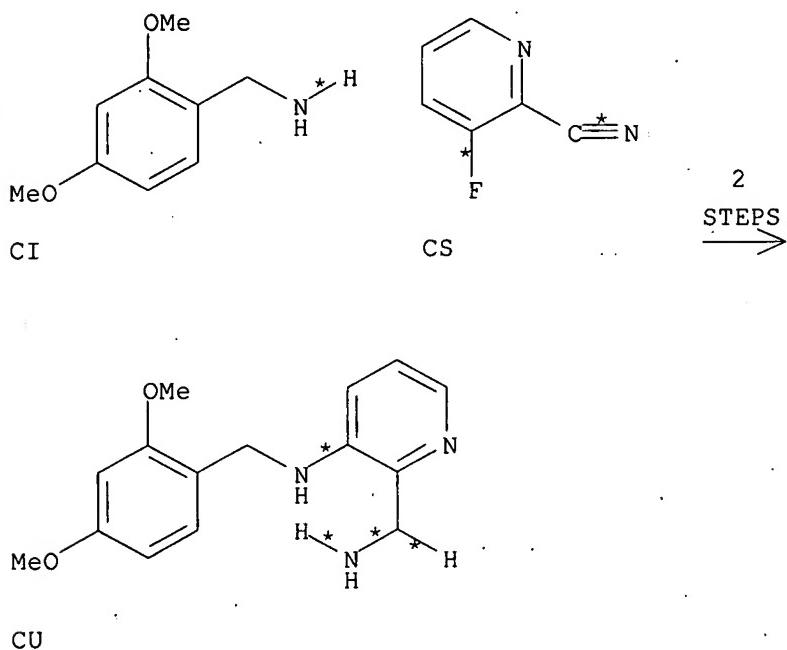
OTHER SOURCE(S): MARPAT 142:240471

GI



AB Benzodiazepine derivs. of formula I [R1 = .H, alkyl, cycloalkyl, aryl, etc.; R2 = H, alkyl, cycloalkyl, aryl, etc.; R3 = H, alkyl, CO<sub>2</sub>H, alkoxy carbonyl; R4 = H, alkyl, cycloalkyl, aryl, etc.; R5 = H, alkyl, cycloalkyl, etc.; n = 1-4; m = 1-9; p = 1-4; W = O, (substituted) NH, (substituted) CH<sub>2</sub>; X = C, S; Y = O, NCONH<sub>2</sub>, etc.; G, J = N, NCH<sub>2</sub>, etc.; Q, T, U, V = CH, N; with provisos] are prepared as antagonists of CGRP receptors, and are useful in the treatment or prevention of diseases in which the CGRP is involved, such as headache, migraine and cluster headache. The invention is also directed to pharmaceutical compns. comprising these compds. and the use of these compds. and compns. in the prevention or treatment of such diseases in which CGRP is involved. Thus, II was prepared in several steps. The prepared compds. had IC<sub>50</sub> values < 50 μM against CGRP receptor.

RX(83) OF 165 COMPOSED OF RX(42), RX(43)  
RX(83) CI + CS ==> CU .



RX(42) RCT CI 20781-20-8, CS 97509-75-6

## STAGE (1)

RGT E 121-44-8 Et3N  
 SOL 127-19-5 AcNMe<sub>2</sub>  
 CON 4 hours, 80 deg C

## STAGE (2)

RGT U 7732-18-5 Water

PRO CT 784155-72-2

RX (43) RCT CT 784155-72-2

10535723

STAGE(1)

RGT CN 16853-85-3 LiAlH4  
SOL 109-99-9 THF  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 0 deg C -> room temperature  
SUBSTAGE(3) 4 hours, room temperature

STAGE(2)

RGT CO 7757-82-6 Na2SO4  
SOL 7732-18-5 Water  
CON room temperature

PRO CU 784155-73-3

L29 ANSWER 3 OF 7 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 141:123579 CASREACT

TITLE: Discovery and Evaluation of Potent P1 Aryl Heterocycle-Based Thrombin Inhibitors

AUTHOR(S): Young, Mary Beth; Barrow, James C.; Glass, Kristen L.; Lundell, George F.; Newton, Christina L.; Pellicore, Janetta M.; Rittle, Kenneth E.; Selnick, Harold G.; Stauffer, Kenneth J.; Vacca, Joseph P.; Williams, Peter D.; Bohn, Dennis; Clayton, Franklin C.; Cook, Jacquelynn J.; Krueger, Julie A.; Kuo, Lawrence C.; Lewis, S. Dale; Lucas, Bobby J.; McMasters, Daniel R.; Miller-Stein, Cynthia; Pietrak, Beth L.; Wallace, Audrey A.; White, Rebecca B.; Wong, Bradley; Yan, Youwei; Nantermet, Philippe G.

CORPORATE SOURCE: Medicinal Chemistry, Pharmacology, Biological Chemistry, Structural Biology, Molecular Systems and Drug Metabolism, Merck Research Laboratories, Merck and Co. Inc., West Point, PA, 19486, USA

SOURCE: Journal of Medicinal Chemistry (2004), 47(12), 2995-3008

CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

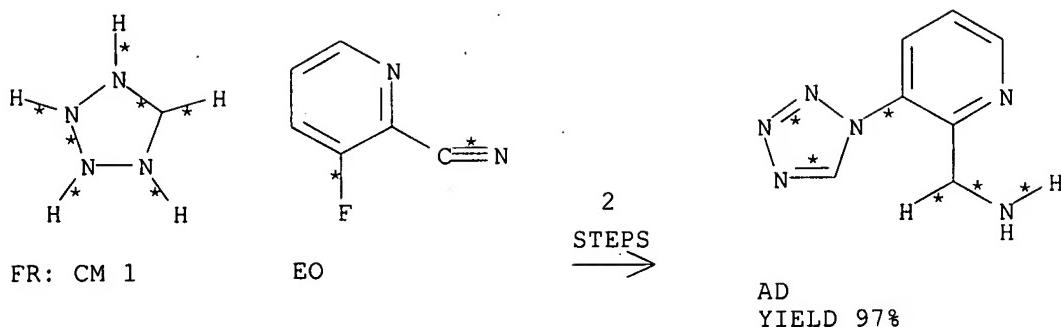
LANGUAGE: English

AB In an effort to discover potent, clin. useful thrombin inhibitors, a rapid analog synthetic approach was used to explore the P1 region. Various benzylamines were coupled to a pyridine/pyrazinone P2-P3 template. One compound, i.e. 2-[6-chloro-3-(2,2-difluoro-2-pyridin-2-yl-ethylamino)-2-oxo-2H-pyrazin-1-yl]-N-(2-[1,2,3]thiadiazol-4-yl-benzyl)acetamide, was found to have a thrombin Ki of 0.84 nM. A study of ortho-substituted five-membered-ring heterocycles was undertaken and subsequently demonstrated that the o-triazole and tetrazole rings were optimal. Combination of these potent P1 aryl heterocycles with a variety of P2-P3 groups produced a compound with an extraordinary thrombin inhibitory activity of 1.4 pM. It is hoped that this potency enhancement in P1 will allow for more diversification in the P2-P3 region to ultimately address addnl. pharmacol. concerns.

RX(158) OF 284 COMPOSED OF RX(84), RX(85)

RX(158) FR + EO ==> AD

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RX (84)      RCT      FR 27988-97-2

STAGE (1)

RGT      FT 2052-49-5 Bu<sub>4</sub>NOH  
SOL      7732-18-5 Water, 68-12-2 DMF

STAGE (2)

RCT      EO 97509-75-6  
CON      4 days, room temperature

PRO      FS 449758-32-1

RX (85)      RCT      FS 449758-32-1  
RGT      CR 1333-74-0 H<sub>2</sub>  
PRO      AD 449756-99-4  
CAT      7440-05-3 Pd  
SOL      64-17-5 EtOH  
CON      overnight, room temperature, 55 psi

REFERENCE COUNT:      22      THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 4 OF 7 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:      141:7024 CASREACT

TITLE:      A novel process for the preparation of 2-aminomethylpyridine derivatives via Ni-catalyzed hydrogenation of 2-cyanopyridine derivatives

INVENTOR(S):      Vangelisti, Manuel

PATENT ASSIGNEE(S):      Bayer Cropscience Sa, Fr.

SOURCE:      Eur. Pat. Appl., 6 pp.

CODEN: EPXXDW

DOCUMENT TYPE:      Patent

LANGUAGE:      English

FAMILY ACC. NUM. COUNT:      1

PATENT INFORMATION:

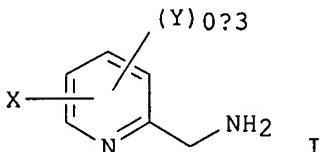
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1422221	A1	20040526	EP 2002-356236	20021120
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK			
WO 2004046114	A1	20040603	WO 2003-EP14892	20031118
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,			

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GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,  
LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO,  
NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ,  
TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW  
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,  
BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,  
ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK,  
TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG  
AU 2003290121 A1 20040615 AU 2003-290121 20031118  
BR 2003014461 A 20050726 BR 2003-14461 20031118  
EP 1565440 A1 20050824 EP 2003-782483 20031118  
EP 1565440 B1 20061220  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK  
CN 1711244 A 20051221 CN 2003-80103328 20031118  
JP 2006508143 T 20060309 JP 2004-552709 20031118  
AT 348811 T 20070115 AT 2003-782483 20031118  
US 2006004206 A1 20060105 US 2005-535723 20050520  
PRIORITY APPLN. INFO.: EP 2002-356236 20021120  
WO 2003-EP14892 20031118

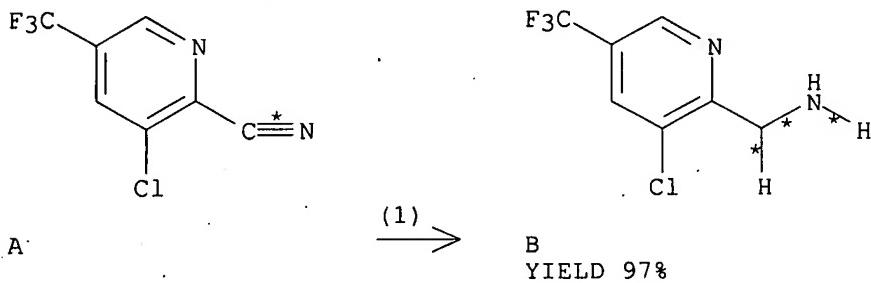
OTHER SOURCE(S): MARPAT 141:7024

GI



AB The invention relates to a process for the preparation of 2-aminomethylpyridine derivs. of formula I [wherein: X is halogen atom; each Y may be the same or different and may be a halogen atom, a halogenoalkyl, an alkoxy carbonyl or an alkylsulfonyl], useful as intermediates for preparation of pesticides. 2-Aminomethyl-3-chloro-5-trifluoromethylpyridine was prepared via Raney Ni-catalyzed hydrogenation of 2-cyano-3-chloro-5-trifluoromethylpyridine with a yield of 97%. The advantages of the proposed preparation of 2-aminomethylpyridine derivs. include the use of Raney nickel catalyst instead of expensive Pd catalyst (the Pd-catalyzed hydrogenation suffers from the disadvantage of dehalogenation reaction; Pd is also very sensitive to catalyst poisons).

RX(1) OF 1      A    ==>    B



Updated Search

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RX(1) RCT A 80194-70-3  
RGT C 1333-74-0 H<sub>2</sub>  
PRO B 175277-74-4  
CAT 7440-02-0 Ni  
SOL 64-19-7 AcOH  
CON SUBSTAGE(1) room temperature -> 40 deg C, pH 7  
SUBSTAGE(2) 2 hours, 40 deg C, 18 bar, pH 7  
NTE Raney nickel used

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 5 OF 7 CASREACT COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 140:272675 CASREACT

TITLE: Development of a Scaleable Synthesis of a 3-Aminopyrazinone Acetamide Thrombin Inhibitor

AUTHOR(S): Ashwood, Michael S.; Alabaster, Ramon J.; Cottrell, Ian F.; Cowden, Cameron J.; Davies, Antony J.; Dolling, Ulf H.; Emerson, Khateeta M.; Gibb, Andrew D.; Hands, David; Wallace, Debra J.; Wilson, Robert D.

CORPORATE SOURCE: Department of Process Research, Merck Sharp and Dohme Research Laboratories, Hoddesdon, Hertfordshire, EN11 9BU, UK

SOURCE: Organic Process Research & Development (2004), 8(2), 192-200

CODEN: OPRDFK; ISSN: 1083-6160

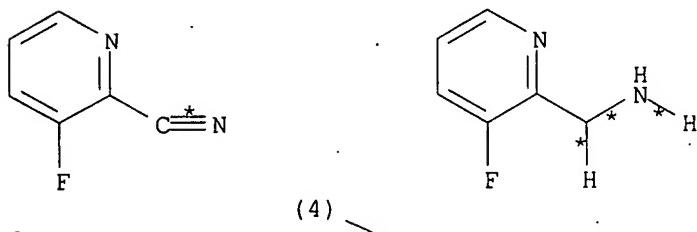
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A scaleable route to 2-{3-[2,2-difluoro-2-(2-pyridyl)ethyl]amino}-6-chloro-2-oxohypyrazinyl-N-[(3-fluoro(2-pyridyl)methyl]acetamide (I) is described in which various scaleup issues were addressed to provide a safe, efficient, and robust route for the preparation of multi-kilo amts. of the compound. The use of expensive and toxic reagents, notably sodium azide, TMS-cyanide, and Deoxo-Fluor, and the need for specialist equipment were overcome in the preparation of the key fluorinated intermediates 2,2-difluoro-2-(2-pyridyl)ethylamine and 2-aminomethyl-3-fluoropyridine. With minimal isolations and through processing of intermediates, the thrombin inhibitor I was isolated in 36% overall yield.

RX(4) OF 84 ...O ==> R...



R  
YIELD 92%

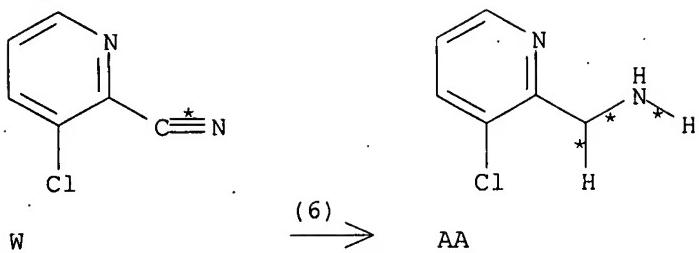
10535723

RX(4) RCT O 97509-75-6  
RGT S 7647-01-0 HCl, T 1333-74-0 H2  
PRO R 312904-49-7  
CAT 7440-05-3 Pd  
SOL 64-17-5 EtOH  
CON 18 hours, 20 deg C, 5 psi  
REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L29 ANSWER 6 OF 7 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 138:198146 CASREACT  
TITLE: Metabolism-Directed Optimization of 3-Aminopyrazinone Acetamide Thrombin Inhibitors. Development of an Orally Bioavailable Series Containing P1 and P3 Pyridines  
AUTHOR(S): Burgey, Christopher S.; Robinson, Kyle A.; Lyle, Terry A.; Sanderson, Philip E. J.; Lewis, S. Dale; Lucas, Bobby J.; Krueger, Julie A.; Singh, Rominder; Miller-Stein, Cynthia; White, Rebecca B.; Wong, Bradley; Lyle, Elizabeth A.; Williams, Peter D.; Coburn, Craig A.; Dorsey, Bruce D.; Barrow, James C.; Stranieri, Maria T.; Holahan, Marie A.; Sitko, Gary R.; Cook, Jacquelynn J.; McMasters, Daniel R.; McDonough, Colleen M.; Sanders, William M.; Wallace, Audrey A.; Clayton, Franklin C.; Bohn, Dennis; Leonard, Yvonne M.; Detwiler, Theodore J., Jr.; Lynch, Joseph J., Jr.; Yan, Youwei; Chen, Zhongguo; Kuo, Lawrence; Gardell, Stephen J.; Shafer, Jules A.; Vacca, Joseph P.  
CORPORATE SOURCE: Departments of Medicinal Chemistry, Biological Chemistry, Drug Metabolism Molecular Systems, Structural Biology and Pharmacology, Merck Research Laboratories, West Point, PA, 19486, USA  
SOURCE: Journal of Medicinal Chemistry (2003), 46(4), 461-473  
CODEN: JMCMAR; ISSN: 0022-2623  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Recent efforts in the field of thrombin inhibitor research have focused on the identification of compds. with good oral bioavailability and pharmacokinetics. In this manuscript we describe a metabolism-based approach to the optimization of the 3-(2-phenethylamino)-6-methylpyrazinone acetamide template which resulted in the modification of each of the three principal components (i.e., P1, P2, P3) comprising this series. As a result of these studies, several potent thrombin inhibitors were identified which exhibit high levels of oral bioavailability and long plasma half-lives.

RX(6) OF 261 ...W ==> AA...

10535723



RX(6) RCT W 38180-46-0  
RGT AB 7664-41-7 NH<sub>3</sub>, AC 1333-74-0 H<sub>2</sub>  
PRO AA 500305-98-6  
CAT 7440-02-0 Ni  
SOL 64-17-5 EtOH  
CON 5 hours, 1 atm  
NTE Raney nickel used  
REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

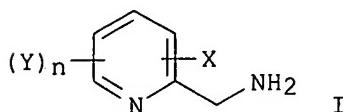
L29 ANSWER 7 OF 7 CASREACT COPYRIGHT 2007 ACS on STN  
ACCESSION NUMBER: 136:200109 CASREACT  
TITLE: Process for preparation of 2-aminomethylpyridines by catalytic hydrogenation of 2-cyanopyridines.  
INVENTOR(S): Dann, Norman; Riordan, Peter Dominic; Amin, Mehul Rasikchandra; Mellor, Michael  
PATENT ASSIGNEE(S): Aventis CropScience SA, Fr.  
SOURCE: PCT Int. Appl., 18 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002016322	A2	20020228	WO 2001-EP10984	20010821
WO 2002016322	A3	20020606		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
EP 1199305	A1	20020424	EP 2001-420128	20010607
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
CA 2415842	A1	20020228	CA 2001-2415842	20010821
AU 200213948	A	20020304	AU 2002-13948	20010821
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R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			

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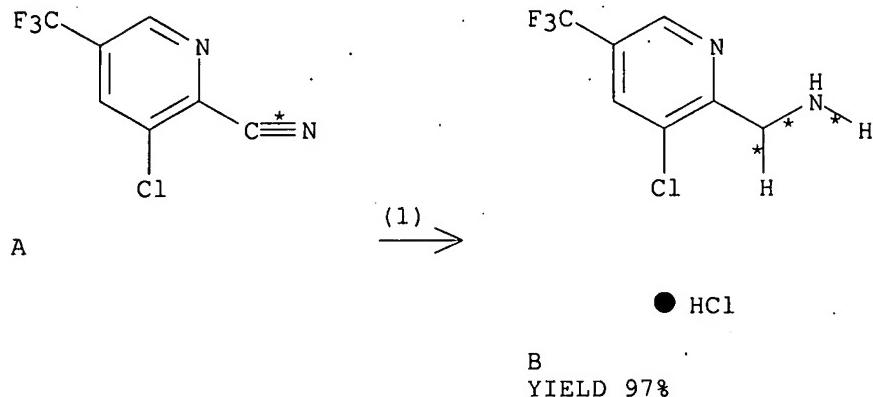
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OTHER SOURCE(S): MARPAT 136:200109  
GI



AB Title compds. (I; X = halo, Y = halo, haloalkyl, alkoxy carbonyl, alkylsulfonyl; n = 0-3) were prepared by catalytic hydrogenation of the corresponding 2-cyano derivs. Thus, 3-chloro-2-cyano-5-trifluoromethylpyridine (preparation given) was hydrogenated in MeOH over Pd/C containing HCl at 1 atmospheric to give 95-97% 2-aminomethyl-3-chloro-5-trifluoromethylpyridine hydrochloride.

RX(1) OF 1 A ==> B



RX(1) RCT A 80194-70-3  
RGT C 1333-74-0 H2, D 7647-01-0 HC1

## Updated Search

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PRO B 326476-49-7  
CAT 7440-05-3 Pd  
SOL 67-56-1 MeOH